Probing Heterogeneous Ice Nucleation on the Muscovite Mica surfaces via Molecular Dynamics Simulations

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Heterogeneous ice nucleation (HIN) has various applications in the field of atmospheric science, cloud modeling, food preservation, and nanotechnology. Muscovite mica is one of the most abundant minerals in the atmosphere and its HIN efficiency has widely been debated. Various experiments and simulations have attempted to correlate the arrangement of water molecules on the mica surface to its ice-nucleating capability, but no clear picture has yet emerged. We present a large-scale molecular dynamics simulation study of the HIN mechanism on the mica (001) basal surface. We show that in the absence of ions, a plane of ice attaches to the mica surface that resembles closely the (20-21) plane of hexagonal ice, resulting in spontaneous freezing at moderate supercooling. This differs from ice nucleation mechanisms that have been observed for other surfaces, which occur via the basal or prism face of ice. A protonated mica surface is found to nucleate ice by the same mechanism. With potassium ions on the mica surface, ice nucleation is disrupted. The connection between the surface morphology of mica and the ice nucleation mechanism is discussed in detail. We found that the arrangement of surface protons and aluminum atoms plays a crucial role in determining mica's HIN efficiency. The simulation analysis is compared with recent experimental results. The effect of finite size systems on the HIN mechanism is also elaborated, which is not taken care of by a recently published study. The results presented here shed new light on the ice nucleation mechanism taken by the muscovite mica surface.